# Computational Method for Determining Peak Locations in an INADEQUATE

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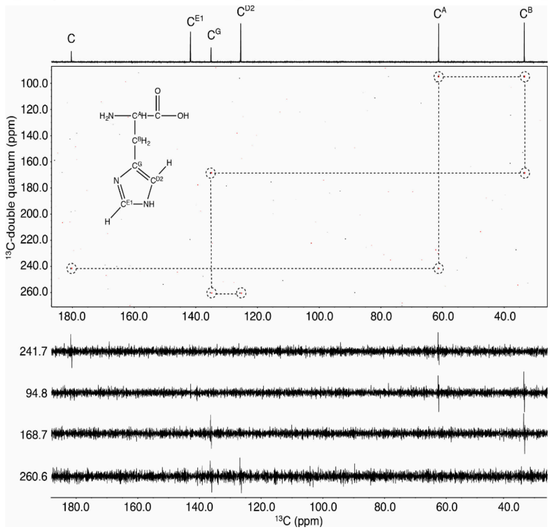
## ABSTRACT

Due to recent advancements in metabolomics, it has become easier for scientists to identify patterns in the chemical structure of compounds using Nuclear Magnetic Resonance (NMR) Spectroscopy. One technique is the 2-D Incredible Natural Abundance Double Quantum Transfer Experiment (INADEQUATE). It is not too difficult to decipher an INADEQUATE spectrum if it contains one or two compounds. However, as the number of compounds increase, it can be challenging and time-consuming to determine the structure of the compound. The purpose of our project is to create a script that can filter any peak list and determine all peak locations.

## BACKGROUND

The Incredible Natural Abundance Double Quantum Transfer Experiment (INADEQUATE) allows us to trace the skeleton of organic compounds using direct carbon-carbon connectives. It is a very powerful experiment in which uses high concentrations of $^{13}C$ atoms and detects only transitions from systems with two spins or more. An example of an INADEQUATE Spectrum is shown to the right.




## REFERENCES

Silverstein, Robert M., Francis X. Webster and David J. Kiemle. Spectrometric Identification of Organic Compounds. Seventh ed. New York: Wiley, 2005.Print.

## SOFTWARE USED

MATLAB
OCEAN MOON NMR VIEW

## ACKNOWLEDGMENTS

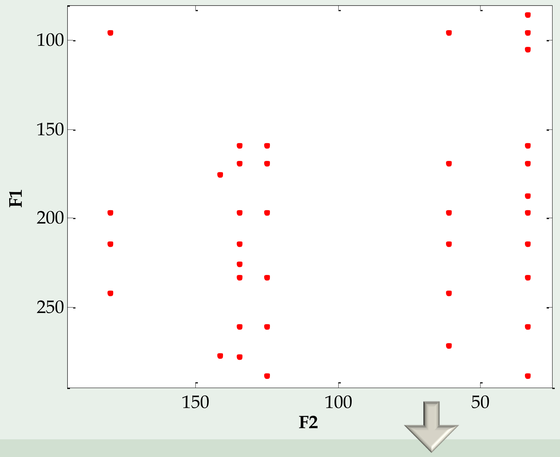
I would like to acknowledge and thank:

The National Magnetic Field Laboratory
University of Florida
Member of the Edison Laboratory
Chaevien Clendinen
Dr. Arthur Edison

My home institution of Claflin University
Dr. Ananda Mondal
Dr. Brent Munsell

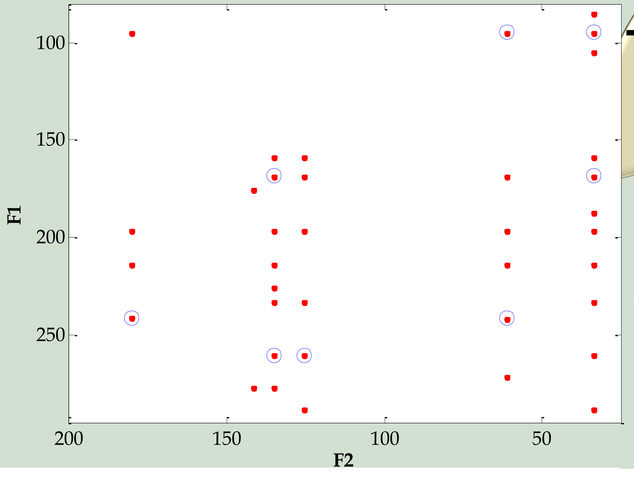
## METHODOLOGY

Figure 1.1 Raw Data of INADEQUATE




The raw data in Figure 1.1: was a mixture that contained L-Histidine. We were able to construct a peak list by retrieving all the data from the F1 and F2 axis. The script is designed to detect two points on the F2 axis and compare it to the data on F1 axis, as shown in Figure 1.3. The script then finds the midpoint between the two peaks on the F2 axis, as shown in Figure 1.3.1. It continues until all the peaks on the peak list have been checked. Once all peaks are checked, then the other formatting is done and the final INADEQUATE spectrum is created, Figure 1.4.

Figure 1.2 The Genuine Crosspeaks on the INADEQUATE



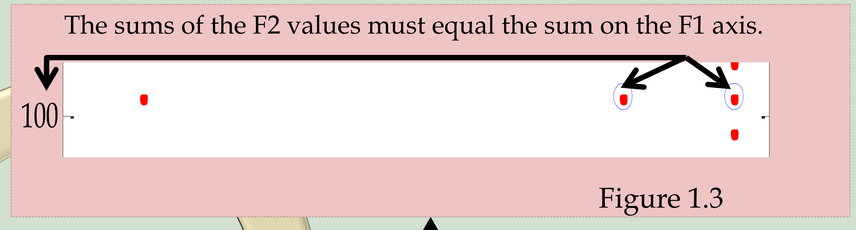




Figure 1.3

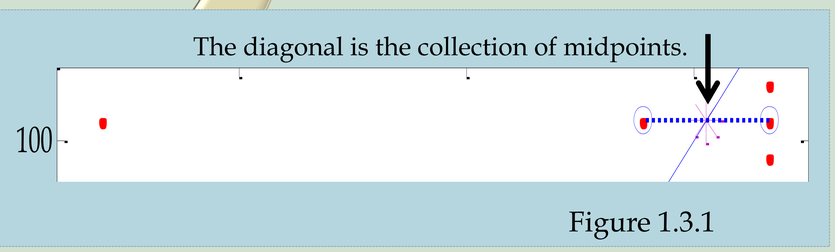



Figure 1.3.1

## RESULTS AND FUTURE WORK

The script was successful in identifying all genuine peak locations for the sample. In addition, it was able to detect and identify all peaks that matched with L-Histidine in the mixture, as shown in Figure 1.4.

We have shown that this script is able to find all the peak locations using a peak list. In the future, we plan to improve the script by just using the raw data itself, instead of retrieving a peak list.

We also plan to expand this script to help make deciphering other 2-D NMR methods more efficient and effective.

Figure 1.4: The INADEQUATE Spectrum